

**The Forming Factors of High Values of  
Superconducting Transition Temperature  $T_c$   
in  $3d$ -Transition Metal Compounds**

**III. Quantum Mechanic Relaxational Model for  
Calculation of the Values of Superconducting  
Transition Temperature  $T_c$**

**Elmira Yuryeva**

Ural State Pedagogical University  
Kosmonavtov av. 26, 620017, Ekaterinburg, Russia  
[yuryeva55@mail.ru](mailto:yuryeva55@mail.ru)

**Anatoliy Yuryev**

Ural Federal University, Mira st. 19, 620002 Ekaterinburg, Russia  
[yurev\\_anatolii@mail.ru](mailto:yurev_anatolii@mail.ru)

Copyright © 2013 Elmira Yuryeva and Anatoliy Yuryev. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

**Abstract**

Within this work is shown that the method of calculation of temperature of loss of stability of an electronic subsystem (ionization temperature) can be used as method of estimation of temperature of transition to a superconducting state in  $3d$ -metal row compounds.

**Keywords:** Quantum mechanic, Relaxational model, Superconducting transition temperature

Although the discovery in 1986 of high-temperature superconductivity (HTSC) in a series of layered copper oxides is now more than twenty years old, it is still actually to establish the microscopic mechanisms of this effect. It may be supposed that the fundamental tenets of the BCS theory [1] are also valid for high-temperature (high- $T_C$ ) superconductors (SC). Yet, it should be admitted that the character of inter atomic bonding in low- and high- $T_C$  superconductors differ essentially [2]. Complete review of the state of the art in superconductivity over the period to 2000 is given in [3].

Recently new data [4, 5] became available on structural distortions of the crystal lattice of high- $T_C$  superconductors near the superconducting transition temperature. So, it was noted in [6] that the presence of structure instability hinders the growth of HTSC transition temperature  $T_C$  in  $\text{HgBa}_2\text{CuO}_{4+\delta}$ . We showed earlier [7] that the mobility of oxygen atoms in the tetragonal high-temperature phase of yttrium-barium ceramic in structure transition to a low-temperature crystalline orthogonal phase is realized already at 80°C, whereas in [8] this value was reduced to room temperature.

In this work we propose the following simple phenomenological model for description the conditions of transition to superconducting state in a complex oxide of 3d-metal compounds.

Assumption 1. We believe that at temperatures below the critical temperature  $T_C$  of the superconducting transition there are free electrons in a specimen, and it is those electrons that determine the electron superconductivity effect. If partial or complete localization of the free electrons on ion cores is possible with temperature growth, this temperature value will be thought to be the temperature, at which a system loses its superconducting properties.

For details we will consider an isolated fragment of the phase of condensed medium (FPCM)  $[A^{k+}B^{l-}]_m^Q$ , where  $Q$  is charge of FPCM, with geometry which corresponds to the geometry of the crystal lattice of a compound that exhibits at temperatures below  $T_C$  property of high-temperature superconductivity.

FPCM acquires the redundant electrical (usually negative), charge  $Q = k - lm$ ,  $k$  is formally defined, i.e. determined under the assumption of a purely ionic bond  $AB$  type, the positive charge of the central metal atom  $A$ ,  $l$  is formally defined charge of the nonmetal atom  $B$  type participating in the formation of the first coordination sphere of the central metal atom  $A$ ,  $m$  is number of atoms of  $B$  type in the first coordination shell of the atom  $A$ .

Assumption 2. The main idea is as follows. Let FPCM in superconducting state is characterized by the number of current carriers  $n$ : FPCM-I became as  $[A^{(n+k)+}B^{l-}]_m^{Q(I)}$  и  $Q(I) = (n+k) - lm$ . In the state when superconducting is absent, i.e. when there is finite electrical resistance, the number of carriers in the FPCM is decreased in a general case by a unity and is becomes equal to  $n-1$ : FPCM-II became as  $[A^{(n-1+k)+}B^{l-}]_m^{Q(II)}$  и  $Q(II) = (n-1+k) - lm$ .

Thus, the temperature, at which a system loses superconducting properties, will be the temperature, at which the difference of energies of both FPCM-I and FPCM-II will be proportional to  $k_B T_C$ .

Assumption 3. We postulate that for the calculation of the temperature of FPCM transition from one crystal or charge state to another state as the amount of energy of FPCM can be used the value of reduced binding energy  $\tilde{E}_{bin}$ , for which the earlier [9] a formula was proposed

$$\tilde{E}_{bin} = \frac{1}{N(a)} \frac{E_{bin}}{N(e)}. \quad (1)$$

Here  $N(a) = \sum_{i=1} Z_i = Z_A + mZ_B$  is the total charge of all the nuclei of the atoms of FPCM;  $Z_i$  is the nuclear charge of the  $i$ -th atom;  $N(e)$  is the number of electrons of FPCM, which in the general case are taken into account for calculation of the electronic structure FPCM;  $E_{bin}$  is FPCM binding energy, calculated for the number of electrons  $N(e)$ . For the calculation of the binding energy required calculations, based on the principles of quantum mechanics. In this regard, our model is a quantum-mechanical model.

Finally the calculation formula is as follows:

$$T_C = \left| \frac{\tilde{E}_{bin}(II) - \tilde{E}_{bin}(I)}{k_B} \right|, \quad (2)$$

where  $\tilde{E}_{bin}(I)$  is reduced binding energy, calculated for  $N(e) - 1$  electrons in FPCM;  $\tilde{E}_{bin}(II)$  is reduced binding energy calculated for  $N(e)$  of the electrons in FPCM;  $k_B$  is Boltzmann constant. This formula has a semi-phenomenological nature and for its utilization is important to find such FPCM, which either sends electron in the conduction band at low temperatures as FPCM-I, or binds it at higher temperatures as FPCM-II.

Assumption 4. We propose to use this approach for the calculation of the transition temperature to the superconducting state, taking into account the two possible mechanisms of electron relaxation in the excited state in the conduction band: the spin-spin and spin-lattice relaxations.

This assumption about the possible influence of the relaxation mechanism for the formation of the superconducting transition temperature values allows us to characterize our model for calculation  $T_C$  as a relaxation model.

In the case where the damping of the spin-lattice relaxation occurs at higher temperature than the damping the spin-spin relaxation, then we accept that the superconducting transition temperature will be determined by the temperature the damping namely the spin-spin relaxation  $T^{el}$ , and then we can assume that  $T_C = T^{el}$ . Precisely in this case we can use the expression (2).

If for the damping of the spin-lattice relaxation is required smaller temperatures  $T^{lat}$  than for the the damping of the spin-spin relaxation  $T^{el}$ , i.e.  $T^{lat} < T^{el}$ , then the lattice can participate in the relaxation process from the initial high to very low temperatures. In the future, this case was not examined by us.

In accordance with the assumptions 3 and 4 the proposed model can be consider as a quantum-mechanical relaxation model and can be used for the actual calculations.

## References

- [1]. J. Bardeen, L.N. Cooper, J.R. Schrieffer, Theory of Superconductivity, Phys. Rev., (105) 1957, 1175 – 1204.
- [2]. M.M. Doria, A.R. de Romaquera, S. Salem-Sugui, Jr., Vanishing of the upper critical field in  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$  from Landau-Ott scaling, Phys. Rev. B., (76) 2007, 052504-1 - 052504-3.
- [3]. V.L. Ginzburg, “Superconductivity: the day before yesterday— yesterday— today— tomorrow”, Phys. Usp., (43) 2000, 573–583.
- [4]. E. Dagotto, Complexibility in Strongly Correlated Electronic Systems, Science, (309) 2005, 257 - 262.
- [5]. S. Smadici, P. Abbamonte, M. Taguchi, Y. Kohsaka, T. Sasagawa, M. Azuma, M. Takano, H. Takagi, Absence of long-ranged charge order in  $\text{Na}_x\text{Ca}_{2-x}\text{CuO}_2\text{Cl}_2$ , Phys. Rev. B, (75) 2007, 075104-1 - 075104-4.
- [6]. B. Dabrowski, Z. Wang, K. Rogaki, J.D. Jorgensen, R.L. Hitterman, J.L. Wagner, B.A. Hunter, P.G. Radaelly, D.G. Hinks, Dependence of superconducting transition temperature on doping and structural distortion of the  $\text{CuO}_2$  planes in  $\text{La}_{2-x}\text{M}_x\text{CuO}_4$  ( $\text{M}=\text{Nd}, \text{Ca}, \text{Sr}$ ), Phys. Rev. Lett., 69 (1996) 1348 – 1351.
- [7]. E.I. Yuryeva,  $X_\alpha$ -DVM modelling of oxygen transport in  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  and  $\text{SrFeO}_3$ , Intern. J. Quantum Chem., (106) 2006, 2290-2296.
- [8]. A.V. Fetisov, E.A. Pastukhov, Phase State of  $\text{YBa}_2\text{Cu}_3\text{O}_\delta$  ( $\delta = 6.7 - 7.4$ ). That has been modified at ambient temperature, Chem. Sustainable Developm., (14) 2006, 395-404
- [9]. È.I. Yurieva, Ab initio modeling of interatomic interactions in  $3\text{C-SiC:M}$ ,  $\text{M}=\text{Cr}, \text{Mn}, \text{Fe}, \text{Co}$ , J. Struct. Chem., (45) 2004, 206 - 213.

**Received: June 12, 2013**